Linear Algebra and its Applications 430 (2009) 924–940

Contents lists available at ScienceDirect

Linear Algebra and its Applications

journal homepage: www.elsevier.com/locate/laa

Simplicity transformations for three-way arrays with symmetric slices, and applications to Tucker-3 models with sparse core arrays

Jorge N. Tendeiro*, Jos M.F. Ten Berge, Henk A.L. Kiers

Department of Psychology, University of Groningen, 9700 AV Groningen, The Netherlands

ARTICLE INFO

Article history:
Received 21 February 2008
Accepted 2 September 2008
Available online 22 November 2008

Submitted by R.A. Brualdi

AMS classification:
15A69

Keywords:
Three-mode component analysis
Candecomp
Parafac
Typical tensorial rank
Tucker transformations
Maximal simplicity
Sparse arrays

ABSTRACT

Tucker three-way PCA and Candecomp/Parafac are two well-known methods of generalizing principal component analysis to three way data. Candecomp/Parafac yields component matrices **A** (e.g., for subjects or objects), **B** (e.g., for variables) and **C** (e.g., for occasions) that are typically unique up to jointly permuting and rescaling columns. Tucker-3 analysis, on the other hand, has full transformational freedom. That is, the fit does not change when **A**, **B**, and **C** are postmultiplied by nonsingular transformation matrices, provided that the inverse transformations are applied to the so-called core array $\underline{\mathbf{G}}$. This freedom of transformation can be used to create a simple structure in **A**, **B**, **C**, and/or in $\underline{\mathbf{G}}$. This paper deals with the latter possibility exclusively. It revolves around the question of how a core array, or, in fact, any three-way array can be transformed to have a maximum number of zero elements. Direct applications are in Tucker-3 analysis, where simplicity of the core may facilitate the interpretation of a Tucker-3 solution, and in constrained Tucker-3 analysis, where hypotheses involving sparse cores are taken into account. In the latter cases, it is important to know what degree of sparseness can be attained as a tautology, by using the transformational freedom. In addition, simplicity transformations have proven useful as a mathematical tool to examine rank and generic or typical rank of three-way arrays. So far, a number of simplicity results have been attained, pertaining to arrays sampled randomly from continuous distributions. These results do not apply to three-way arrays with symmetric slices in one direction. The present paper offers a number of simplicity results for arrays with symmetric slices of order $2 \times 2, 3 \times 3$ and 4×4. Some generalizations to higher orders

* Corresponding author.
E-mail addresses: j.n.tendeiro@rug.nl (J.N. Tendeiro), j.m.f.ten.berge@rug.nl (J.M.F. Ten Berge), h.a.l.kiers@rug.nl (H.A.L. Kiers).

doi:10.1016/j.laa.2008.09.020

are also discussed. As a mathematical application, the problem of determining the typical rank of $4 \times 3 \times 3$ and $5 \times 3 \times 3$ arrays with symmetric slices will be revisited, using a sparse form with only eight out of 36 elements nonzero for the former case and 10 out of 45 elements nonzero for the latter one, that can be attained almost surely for such arrays. The issue of maximal simplicity of the targets to be presented will be addressed, either by formal proofs or by relying on simulation results.

1. Introduction

Two of the most popular methods of component analysis for three-way arrays are Candecomp/Parafac, henceforth CP [1,3], and Tucker three-way PCA [17], henceforth 3PCA. For a three-way data array $\underline{\mathbf{X}}$ of format $I \times J \times K$, CP yields component matrices $\mathbf{A}(I \times R)$, $\mathbf{B}(J \times R)$, and $\mathbf{C}(K \times R)$, such that $\sum_{k=1}^{K} tr(\mathbf{E}_k'\mathbf{E}_k)$ is minimized in the decomposition

$$\underline{\mathbf{X}} = \sum_{r=1}^{R} (\mathbf{a}_r \circ \mathbf{b}_r \circ \mathbf{c}_r) + \underline{\mathbf{E}}, \tag{1}$$

where $\mathbf{a}_r$, $\mathbf{b}_r$, $\mathbf{c}_r$ are columns r of $\mathbf{A}, \mathbf{B}$, and $\mathbf{C}$, respectively, and $\mathbf{E}_k$ denotes the kth slice of order $I \times J$ of the residual array $\underline{\mathbf{E}}$. It can be seen that an R-component CP solution approximates the data as the sum of R outer products of the form $(\mathbf{a}_r \circ \mathbf{b}_r \circ \mathbf{c}_r)$, $r = 1, \ldots, R$. Equivalently, each frontal slice $\mathbf{X}_k$ of $\underline{\mathbf{X}}$ is decomposed as

$$\mathbf{X}_k = \mathbf{A}\mathbf{C}_k\mathbf{B}' + \mathbf{E}_k, \tag{2}$$

where $\mathbf{C}_k$ is the diagonal matrix holding the elements from row k of $\mathbf{C}$.

Like CP, 3PCA approximates the data array as a sum of outer products of columns of $\mathbf{A}(I \times P)$, $\mathbf{B}(J \times Q)$, and $\mathbf{C}(K \times R)$, but now every outer product of one of the P columns of $\mathbf{A}$, one of the Q columns of $\mathbf{B}$, and one of the R columns of $\mathbf{C}$ is involved, with P, Q, and R possibly different. In addition, each of these PQR outer products is weighted when it enters the sum. The weights are collected in the so-called core array $\underline{\mathbf{G}}$ of format $P \times Q \times R$. Specifically, 3PCA minimizes the function $\sum_{k=1}^{K} tr(\mathbf{E}_k'\mathbf{E}_k)$ in the decomposition

$$\underline{\mathbf{X}} = \sum_{p=1}^{P}\sum_{q=1}^{Q}\sum_{r=1}^{R} g_{pqr}(\mathbf{a}_p \circ \mathbf{b}_q \circ \mathbf{c}_r) + \underline{\mathbf{E}}, \tag{3}$$

where $\mathbf{a}_p, \mathbf{b}_q, \mathbf{c}_r$ are columns p, q, r of $\mathbf{A}, \mathbf{B}$, and $\mathbf{C}$, respectively, and g_{pqr} are entries from $\underline{\mathbf{G}}$. Equivalently, 3PCA can be expressed as

$$\mathbf{X}_k \approx \mathbf{A}\left(\sum_{r=1}^{R} c_{kr}\mathbf{G}_r\right)\mathbf{B}', \quad k = 1, 2, \ldots, K, \tag{4}$$

where $\mathbf{X}_k$ and $\mathbf{G}_r$ denote frontal slices of $\underline{\mathbf{X}}$ and $\underline{\mathbf{G}}$, respectively. The parameters are estimated by minimizing the sum of squared residuals for fixed numbers of components in each mode [7].

Under mild conditions, a solution for CP is essentially unique [4,8,9]. That is, only joint permutations and rescaling of columns of $\mathbf{A}$, $\mathbf{B}$ and $\mathbf{C}$ will leave the fitted part of the solution unaltered. In 3PCA, on the other hand, there is no such uniqueness. In fact, the core array can be transformed in the three directions, as long as the inverse transformations are applied to the component matrices. Specifically, the slabs $\mathbf{G}_1, \ldots, \mathbf{G}_R$ can be transformed to $\mathbf{G}_1^*, \ldots, \mathbf{G}_R^*$ by means of the *Tucker transformation*

$$\mathbf{G}_l^* = \mathbf{S}'\left(\sum_{r=1}^{R} u_{rl}\mathbf{G}_r\right)\mathbf{T}, \quad l = 1, 2, \ldots, R, \tag{5}$$

where $\mathbf{S}$, $\mathbf{T}$, and $\mathbf{U}$, holding elements u_{rl}, are nonsingular, provided that the component matrices are counter-transformed into $\mathbf{A}^* = \mathbf{A}(\mathbf{S}')^{-1}$, $\mathbf{B}^* = \mathbf{B}(\mathbf{T}')^{-1}$ and $\mathbf{C}^* = \mathbf{C}(\mathbf{U}')^{-1}$ [12,17]. Expression (5) can also be written as

$$\mathbf{G}^*_{\text{Vec}} = (\mathbf{T}' \otimes \mathbf{S}')\mathbf{G}_{\text{Vec}}\mathbf{U}, \tag{6}$$

where $\mathbf{G}_{\text{Vec}} = [\text{Vec}(\mathbf{G}_1)|\cdots|\text{Vec}(\mathbf{G}_R)]$ is a vectorised version of $\underline{\mathbf{G}}$, and $\mathbf{G}^*_{\text{Vec}}$ is defined analogously.

One of the problems that are often associated to 3PCA is the difficulty to interpret a solution. The main reason is that the solution involves so many triplets of components. The number of these triplets is the number of relevant nonzero entries in the core array. This situation can be improved if it is possible to transform the core array so that it holds as many zero entries as possible. Such a "simple" core will decrease the number of joint impacts of triples of components from **A**, **B** and **C**, which may facilitate the interpretation. This is a first reason for considering simplicity transformations for core arrays.

Results on simplicity transformations may also be useful to distinguish between tautologies and non-trivial models. Often, researchers impose constraints on the core, based on theory. Once it is proven that a certain simple form is achievable almost surely (via Tucker transformations) for arrays of a given format, then that simple form adds nothing new as a model. The theory is then beyond falsification, and the researcher needs to impose more or different constraints in order to construct a meaningful model.

Apart from being useful for applied 3PCA with or without constraints on the core, transformations to simplicity also may serve as a tool itself for the mathematical study of three-way arrays. For instance, Ten Berge and Kiers [13] and Ten Berge [14] have given results on typical rank (over the real field) of array formats that became obvious after certain simplicity transformations. It is important to note that, although an array is altered when Tucker transformations are used, the rank remains unaffected. This means that one has the freedom to transform an array by Tucker transformations without affecting its rank.

2. Symmetry preserving Tucker transformations

Simplicity transformations for three-way arrays have received considerable attention, e.g. Kiers [5,6], Murakami et al. [10], Ten Berge and Kiers [13], Ten Berge et al. [15], and Rocci and Ten Berge [12]. However, whatever closed-form simplicity results have been obtained, they apply to arrays the elements of which are randomly sampled from a continuous distribution. In practice, data sets frequently contain symmetric slices. For such cases the above results do not hold. Research on simplicity for arrays that have *symmetric* slices in one direction is still absent. The present paper offers simplicity results for the latter type of array.

From now on we assume that $\underline{\mathbf{X}}$ is an $I \times I \times K$ array with K symmetric frontal slices $\mathbf{X}_k$ of order $I \times I, k = 1, \ldots, K$. We assume that these slices are linearly independent, otherwise, we transform the superfluous slices to zero via a suitable transformation (5), reducing the dimensionality of the problem. Because the space of real symmetric matrices of order $I \times I$ has dimension $I(I+1)/2$, the number K of symmetric slices to consider will not exceed $K_{\max} = I(I+1)/2$.

We will usually work under the assumption that $\underline{\mathbf{X}}$ is randomly sampled from a continuous distribution, with the constraint that slices are symmetric in one direction. Phenomena that arise "almost surely" are those that arise with probability one under this circumstance.

We are looking for symmetry-preserving transformations of $\underline{\mathbf{X}}$ which yield an array $\underline{\mathbf{H}}$ with a large number of zero elements. So our goal is to determine nonsingular matrices **S**, **U** such that

$$\mathbf{H}_l = \mathbf{S}' \left(\sum_{k=1}^{K} u_{kl} \mathbf{X}_k \right) \mathbf{S}, \quad l = 1, 2, \ldots, K, \tag{7}$$

where u_{kl} is an element of **U**, has as many zero entries as possible. The number of nonzero entries in $\underline{\mathbf{H}}$ will be referred to as the *weight* of $\underline{\mathbf{H}}$.

It may be noted that we have tacitly assumed in (7) that **S** and **T** of (5) can be constrained to be equal. In fact, this is a simplification, because symmetry preserving transformations with **S** and **T** different do exist. However, this is possible only for two-slice arrays. Moreover, setting **S** and **T** equal has not been detrimental at all in our search for transformations that minimize the weight of arrays.

3. A symmetric version of the orthogonal complement method

Rocci and Ten Berge [12] have developed the so-called orthogonal complement method (henceforth OCM), which permits transforming an array to simple form by using the previously known simplicity transformation of a so-called complementary array. For instance, the seven frontal slices of a $3 \times 3 \times 7$ array $\underline{\mathbf{X}}$ form a 7-dimensional subspace in 9-space, and a complementary array $\underline{\mathbf{X}}^{\mathrm{c}}$ would be any $3 \times 3 \times 2$ array, the slices of which are linearly independent, and trace-orthogonal to the seven slices of $\underline{\mathbf{X}}$. OCM is based on the observation that transformations that simplify $\underline{\mathbf{X}}^{\mathrm{c}}$ may also be used to simplify $\underline{\mathbf{X}}$ itself. For instance, suppose $\underline{\mathbf{X}}^{\mathrm{c}}$ can be transformed to contain two diagonal 3×3 matrices. The subspace spanned by the seven slices of $\underline{\mathbf{X}}$ contains one diagonal matrix and six matrices having just one nonzero element. Finding the linear combinations that produce those seven matrices in a known subspace is easy, which means that the OCM will transform $\underline{\mathbf{X}}$ into an array that has 54 zero elements out of 63.

The OCM has played a key role in obtaining some important results of this paper. However, to be useful in the present context, it needed to be adjusted in two respects. First, the dimensionality of the space of $I \times I$ matrices is I^2 in general, but it is only $I(I+1)/2$ in case of symmetry. So $\underline{\mathbf{X}}$ can be written in a slice-wise vectorised version $\mathbf{X}_{\mathrm{Vec}} = [\mathrm{Vec}(\mathbf{X}_1)|\cdots|\mathrm{Vec}(\mathbf{X}_K)]$ of order $(1/2I(I+1)) \times K$. Second, we need to constrain the transformations to have $\mathbf{S}$ and $\mathbf{T}$ equal. This amounts to the following general setup of OCM for symmetric slice arrays:

Step 1. Compute an orthogonal complement of $\mathbf{X}_{\mathrm{Vec}}$, say $\mathbf{X}^{\mathrm{c}}_{\mathrm{Vec}}$.

Step 2. Compute $\mathbf{H}^{\mathrm{c}}_{\mathrm{Vec}} = (\mathbf{S}^{-1} \otimes \mathbf{S}^{-1})\mathbf{X}^{\mathrm{c}}_{\mathrm{Vec}}\mathbf{V}$ in such a way that $\mathbf{H}^{\mathrm{c}}_{\mathrm{Vec}}$ is in simple form.

Step 3. Compute a simple orthogonal complement of $\mathbf{H}^{\mathrm{c}}_{\mathrm{Vec}}$, say $\mathbf{H}_{\mathrm{Vec}}$.

Step 4. Find the matrix $\mathbf{U}$ such that $\mathbf{H}_{\mathrm{Vec}} = (\mathbf{S}' \otimes \mathbf{S}')\mathbf{X}_{\mathrm{Vec}}\mathbf{U}$. Array $\underline{\mathbf{H}}$, reconstructed from $\mathbf{H}_{\mathrm{Vec}}$, is the simple form found for $\underline{\mathbf{X}}$.

In the next sections, simplicity results for various array formats will be presented. We will denote the array to be simplified by $\underline{\mathbf{X}}$, with symmetric frontal slices $\mathbf{X}_1, \ldots, \mathbf{X}_K$. The simple form to be obtained from $\underline{\mathbf{X}}$ will be denoted by $\underline{\mathbf{H}}$, with symmetric frontal slices $\mathbf{H}_1, \ldots, \mathbf{H}_K$.

We start with the case where the set of symmetric slices in an array is space-filling.

4. Simplifying symmetric slice $I \times I \times K_{\max}$ arrays

When we have the maximum number of linearly independent symmetric frontal slices, the set of the frontal slices forms a basis for the space of symmetric $I \times I$ matrices. Denote the ith column of $\mathbf{I}_I$ by $\mathbf{e}_i$. A simple basis for the same space is formed by matrices $\mathbf{e}_i\mathbf{e}_i'$ for $i = 1, 2, \ldots, I$, and $(\mathbf{e}_i\mathbf{e}_j' + \mathbf{e}_j\mathbf{e}_i')$ for $1 \leqslant i < j \leqslant I$ [11]. For example, when $I = 3$ the basis is

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix},$$
$$\begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}. \tag{8}$$

Therefore, there is a nonsingular $K_{\max} \times K_{\max}$ matrix $\mathbf{U}$ such that $\mathbf{H}_l = \sum_{k=1}^{K_{\max}} u_{kl}\mathbf{X}_k, l = 1, 2, \ldots, K_{\max}$, where the matrices $\mathbf{H}_l$ represent the elements of the simple basis. That is, $\underline{\mathbf{H}}$ holds the elements of the simple basis as frontal symmetric slices. This simple form has weight (number of nonzero elements) I^2, which means that the proportion of nonzero elements is $1/K_{\max} = 2/(I(I+1))$. Clearly, the relative weight gets smaller as the size of the array increases.

This simple form for the $I \times I \times K_{\max}$ symmetric slice array is also useful when we are dealing with tall $I \times I \times K$ arrays, i.e., with $K > K_{\max}$. In this case the frontal slices are linearly dependent. We start by performing a suitable slice mix in order to set the slices in excess to zero, thus we may reduce the number of frontal slices. When $K_{\max}$ linearly independent slices remain, then the above simplification is possible.

5. Simplifying symmetric slice 2 × 2 × K arrays

When $\underline{\mathbf{X}}$ is a $2 \times 2 \times K$ array, there are three cases to consider, that is, we have $K = 1, 2$, or 3. The $2 \times 2 \times 3$ case was already dealt with before ($K_{\max} = 3$). In the $2 \times 2 \times 1$ case there is merely a symmetric matrix $\mathbf{X}$ of order 2. Computing the eigenvalue decomposition $\mathbf{X} = \mathbf{KDK}'$ we get $\mathbf{K}'\mathbf{XK} = \mathbf{D}$. Rescaling $\mathbf{D}$ to make one of its entries unity, we conclude that the diagonal matrix

$$\begin{bmatrix} 1 & 0 \\ 0 & \alpha \end{bmatrix} \tag{9}$$

is a weight 2 simple form for $\mathbf{X}$. An alternative simple form for $\mathbf{D}$ with the same weight is possible if its diagonal entries, say d_1 and d_2, have opposite signs, namely,

$$\mathbf{S}'\mathbf{DS} = \begin{bmatrix} 0 & 2d_1 \\ 2d_1 & 0 \end{bmatrix} \tag{10}$$

with $\mathbf{S} = \begin{bmatrix} 1 & 1 \\ k & -k \end{bmatrix}$ and $k^2 = -(d_1/d_2)$. So $\mathbf{X}$ can be transformed into $\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$ (after rescaling (10)) when the eigenvalues of $\mathbf{X}$ have opposite signs.

For a $2 \times 2 \times 2$ array $\underline{\mathbf{X}} = [\mathbf{X}_1|\mathbf{X}_2]$, the simple form can be computed using the OCM, since $2 \times 2 \times 2$ is complementary to $2 \times 2 \times 1$. It is straightforward that a simple form which is complementary to (9) is given by

$$\left[\begin{array}{cc|cc} \alpha & 0 & 0 & 1 \\ 0 & -1 & 1 & 0 \end{array}\right]. \tag{11}$$

If the orthogonal complement of $\underline{\mathbf{X}}$ has eigenvalues with different signs (that is, if α in (9) is negative), then $\underline{\mathbf{X}}^{\mathrm{c}}$ can be simplified as in (10), entailing the complementary array

$$\left[\begin{array}{cc|cc} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{array}\right]. \tag{12}$$

Any array derived from (12) via a Tucker transformation such that one of the slices is invertible, say $\mathbf{X}_1$, will have an $\mathbf{X}_1^{-1}\mathbf{X}_2$ with real eigenvalues only. Conversely, a $2 \times 2 \times 2$ symmetric array $\underline{\mathbf{X}} = [\mathbf{X}_1|\mathbf{X}_2]$ such that $\mathbf{X}_1^{-1}\mathbf{X}_2$ has only real eigenvalues can always be simultaneously diagonalized as in (12), thus implying an orthogonal complement matrix with one eigenvalue positive and one negative.

To sum up, a weight 4 simple form for a $2 \times 2 \times 2$ symmetric array is almost surely possible. If $\underline{\mathbf{X}}^{\mathrm{c}}$ has both a positive and a negative eigenvalue, or equivalently, if $\mathbf{X}_1^{-1}\mathbf{X}_2$ has real eigenvalues, then a weight 2 simple target is possible.

6. Simplifying symmetric slice 3 × 3 × K arrays

For $3 \times 3 \times K$ arrays, $K_{\max} = 6$. We will search simplicity for cases $K = 1, 2, 4, 5$. Note that the case $K_{\max} = 6$ has already been solved. The case $K = 3$ remains an open issue and is not covered in the present paper.

The $3 \times 3 \times 1$ array (=matrix) can be diagonalized using its eigenvalue decomposition, say $\mathbf{D} = \mathrm{diag}(d_1, d_2, d_3)$. An alternative simple form with the same weight is possible if there is a pair of d_{i}'s with opposite signs, in the same manner as was done to deduce (10). So, if $d_2d_3 < 0$ then

$$\mathbf{S}'\mathbf{DS} = \begin{bmatrix} d_1 & 0 & 0 \\ 0 & 0 & 2d_2 \\ 0 & 2d_2 & 0 \end{bmatrix}, \tag{13}$$

with $\mathbf{S} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 1 \\ 0 & k & -k \end{bmatrix}$ and $k^2 = -(d_2/d_3)$.

The array format $3 \times 3 \times 5$ is complementary to $3 \times 3 \times 1$. We can therefore simplify a $3 \times 3 \times 5$ symmetric array $\underline{\mathbf{X}}$ using the OCM and the known simple form for the $3 \times 3 \times 1$ complementary array

$\underline{\mathbf{X}}^c$. Matrix $\underline{\mathbf{X}}^c$ can always be diagonalized, which in terms of the orthogonal complement means that the following weight 10 simple form is always possible:

$$\left[\begin{array}{ccc|ccc|ccc|ccc|ccc} 1 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & \alpha & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & \beta & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 \end{array}\right]. \tag{14}$$

When $\underline{\mathbf{X}}^c$ has a pair of eigenvalues with opposite signs, then it can be simplified into form (13), which leads to a weight 9 simple form,

$$\left[\begin{array}{ccc|ccc|ccc|ccc|ccc} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & \alpha & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 \end{array}\right]. \tag{15}$$

To sum up, a $3 \times 3 \times 5$ symmetric array can almost surely be simplified into the weight 10 simple array (14). In the special case that the orthogonal complement of $\underline{\mathbf{X}}$ has eigenvalues of both signs, then the weight 9 target (15) is possible. This is the reason why (13) is to be preferred to the diagonal form for the $3 \times 3 \times 1$ case, whenever possible.

Next, we deal with the $3 \times 3 \times 2$ case $\underline{\mathbf{X}} = [\mathbf{X}_1|\mathbf{X}_2]$. Define $\mathbf{M} = \mathbf{X}_1^{-1}\mathbf{X}_2$. We divide our analysis in two cases, depending on the number of complex eigenvalues in $\mathbf{M}$.

- **M has all eigenvalues real**

In this case, array $\underline{\mathbf{X}}$ has rank 3 [16], and there is a CP-solution $\mathbf{X}_k = \mathbf{A}\mathbf{C}_k\mathbf{A}'$ $(k = 1, 2)$, where $\mathbf{A}$ is nonsingular and $\mathbf{C}_k$ is diagonal. So we can write $\mathbf{C}_k = \mathbf{A}^{-1}\mathbf{X}_k(\mathbf{A}^{-1})'$, which is a way of diagonalizing both slices of $\underline{\mathbf{X}}$. Note that $\mathbf{M} = \mathbf{X}_1^{-1}\mathbf{X}_2 = (\mathbf{A}')^{-1}(\mathbf{C}_1^{-1}\mathbf{C}_2)\mathbf{A}'$, which is an eigenvalue decomposition of $\mathbf{M}$. Therefore, an easy way to perform the double diagonalization is to compute the eigendecomposition $\mathbf{M} = \mathbf{K}\mathbf{L}\mathbf{K}^{-1}$, so $\mathbf{A} = (\mathbf{K}^{-1})'$, and compute $[\mathbf{K}'\mathbf{X}_1\mathbf{K}|\mathbf{K}'\mathbf{X}_2\mathbf{K}] = [\mathbf{C}_1|\mathbf{C}_2]$.

Almost surely, $\mathbf{C}_1^{-1}\mathbf{C}_2$ has a pair of distinct diagonal elements, say c_1 and c_2. Array $[\mathbf{C}_1|\mathbf{C}_2]$ may be transformed to $[\mathbf{C}_2 - c_1\mathbf{C}_1| - \mathbf{C}_2 + c_2\mathbf{C}_1]$, which has both slices diagonal of rank two. Notice that the slice mix that was performed consists of a nonsingular transformation in the third direction. So we conclude that a possible weight 4 simple form for the $3 \times 3 \times 2$ symmetric array, in the case when $\mathbf{M}$ has all three eigenvalues real, is

$$\left[\begin{array}{ccc|ccc} 0 & 0 & 0 & \beta & 0 & 0 \\ 0 & \alpha & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 1 \end{array}\right]. \tag{16}$$

When all eigenvalues are real, this simplification can be generalized to any array $\underline{\mathbf{X}} = [\mathbf{X}_1|\mathbf{X}_2]$ holding two symmetric slices of order $I \times I$. The obtained simple form will have weight $(2I - 2)$.

We shall now show how to get a simple form with weight 5. Although for the $3 \times 3 \times 2$ case this means a loss of simplicity, it will be useful for the complementary $3 \times 3 \times 4$ array. We start by considering array $[\mathbf{C}_1|\mathbf{C}_2 - c\mathbf{C}_1]$, where c is an eigenvalue of $\mathbf{C}_1^{-1}\mathbf{C}_2$. If all eigenvalues of $\mathbf{C}_1^{-1}\mathbf{C}_2$ are distinct (this happens almost surely), then for at least one of the eigenvalues, say c, we have that $\mathbf{C}_2 - c\mathbf{C}_1$ will be diagonal, of rank 2, holding two entries with opposite signs in the diagonal. Rescaling both frontal slices of $[\mathbf{C}_1|\mathbf{C}_2 - c\mathbf{C}_1]$ allows us to get the form

$$\left[\begin{array}{ccc|ccc} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & a & 0 & 0 & 1 & 0 \\ 0 & 0 & b & 0 & 0 & c \end{array}\right] \tag{17}$$

with $c < 0$. Entry c may be set to -1 by pre- and postmultiplying both slices by $\operatorname{diag}\left(1, 1, \frac{1}{\sqrt{|c|}}\right)$. Subtract $(a - b)/2$ times the second slice from the first slice to get

$$\left[\begin{array}{ccc|ccc} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & d & 0 & 0 & 1 & 0 \\ 0 & 0 & d & 0 & 0 & -1 \end{array}\right] \tag{18}$$

with $d = (a + b)/2$. Next, pre- and postmultiplying both slices by $\begin{bmatrix} 1 & 0 & 0 \\ 0 & \sqrt{0.5} & \sqrt{0.5} \\ 0 & \sqrt{0.5} & -\sqrt{0.5} \end{bmatrix}$ leads to

$$\left[\begin{array}{ccc|ccc} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & d & 0 & 0 & 0 & 1 \\ 0 & 0 & d & 0 & 1 & 0 \end{array}\right]. \tag{19}$$

A final rescaling of the first slice allows us to conclude that the following simple form is always possible:

$$\left[\begin{array}{ccc|ccc} -\alpha & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 1 & 0 \end{array}\right] \tag{20}$$

with α nonzero. This form will be of use when deriving a simple form for the $3 \times 3 \times 4$ case.

It can be concluded that, for the $3 \times 3 \times 2$ array when $\mathbf{M}$ has all eigenvalues real, both the form (16) and the form (20) are almost surely possible. Form (20) will appear useful later, to derive simplicity for the complementary $3 \times 3 \times 4$ format.

• **M has one pair of complex eigenvalues**

Assume that in the eigenvalue decomposition $\mathbf{M} = \mathbf{KLK}^{-1}$ the real eigenvalue is $\mathbf{L}(1,1)$. Consider $\mathbf{S}_1 = [\mathbf{k}_1|\ \mathrm{real}(\mathbf{k}_2)|\ \mathrm{imag}(\mathbf{k}_2)]$, where $\mathbf{k}_i$ is the ith column of $\mathbf{K}$. Then [18]

$$[\mathbf{S}_1'\mathbf{X}_1\mathbf{S}_1|\mathbf{S}_1'\mathbf{X}_2\mathbf{S}_1] = \left[\begin{array}{ccc|ccc} a & 0 & 0 & d & 0 & 0 \\ 0 & b & c & 0 & e & f \\ 0 & c & -b & 0 & f & -e \end{array}\right]. \tag{21}$$

Subtracting (d/a) times the first slice from the second, and then rescaling the second slice by the inverse of entry (2,2) yields the form

$$[\mathbf{Y}_1|\mathbf{Y}_2] = \left[\begin{array}{ccc|ccc} a & 0 & 0 & 0 & 0 & 0 \\ 0 & b & c & 0 & 1 & f_1 \\ 0 & c & -b & 0 & f_1 & -1 \end{array}\right] \tag{22}$$

Define $\mathbf{S}_2 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & -s \\ 0 & s & 1 \end{bmatrix}$ for $s = f_1 + \sqrt{f_1^2 + 1}$, then

$$[\mathbf{S}_2'\mathbf{Y}_1\mathbf{S}_2|\mathbf{S}_2'\mathbf{Y}_2\mathbf{S}_2] = \left[\begin{array}{ccc|ccc} a_1 & 0 & 0 & 0 & 0 & 0 \\ 0 & b_1 & c_1 & 0 & 0 & f_2 \\ 0 & c_1 & -b_1 & 0 & f_2 & 0 \end{array}\right]. \tag{23}$$

A final linear combination of both slices allows us to have $c_1 = 0$. Therefore, a simple form obtained after a final rescaling is

$$\left[\begin{array}{ccc|ccc} -\alpha & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 & 1 & 0 \end{array}\right]. \tag{24}$$

The overall conclusion for a general $3 \times 3 \times 2$ symmetric slice array is that a weight 5 simple form is always possible, see (20) and (24). In the case when $\mathbf{X}_1^{-1}\mathbf{X}_2$ has all eigenvalues real, the weight 4 form (16) has the smallest possible weight.

We will now apply the OCM to simplify the $3 \times 3 \times 4$ array by using the known simple form of the $3 \times 3 \times 2$ array. It is easy to verify that both (20) and (24) admit as an orthogonal complement an array with form

$$\left[\begin{array}{ccc|ccc|ccc|ccc} 1 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 \\ 0 & \alpha & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \delta\alpha & 0 & 0 & 0 & 1 & 0 & 0 \end{array}\right], \tag{25}$$

where α has the same meaning as in (20) and (24), and $\delta = 1$ in the first case and -1 in the second case. So almost surely a $3 \times 3 \times 4$ symmetric slice array can be simplified to a weight 8 simple form. Interestingly, if we had used (16) as the simple array form for the orthogonal complement (in the real eigenvalue situation), we would have obtained a weight 9 array as simple form for $\underline{\mathbf{X}}$, less simple than (25).

There is still one case left, the $3 \times 3 \times 3$ symmetric slice array. Although this array format seems to allow a simple pattern of weight 9 more often than not, a formal proof of this has evaded us.

7. Simplifying symmetric slice $4 \times 4 \times K$ arrays

In the $4 \times 4 \times K$ case we have $K_{\max} = 10$. So the $4 \times 4 \times 10$ case has been solved. We present simple forms for formats $4 \times 4 \times 1$ and $4 \times 4 \times 2$, as well as their complementary formats $4 \times 4 \times 9$ and $4 \times 4 \times 8$, respectively. The remaining cases are still open.

Arrays (=matrices) of order $4 \times 4 \times 1$ can be diagonalized by means of the eigenvalue decomposition. This means that $\mathbf{D} = \operatorname{diag}(d_1, d_2, d_3, d_4)$, the diagonal matrix holding eigenvalues, is always a possible simple form for the array. Alternative forms, specially useful for the $4 \times 4 \times 9$ complement, may be possible using the same process that was used to obtain (10) for the $2 \times 2 \times 1$ case. Specifically, we may attain the forms

$$\begin{bmatrix} d_1 & 0 & 0 & 0 \\ 0 & d_2 & 0 & 0 \\ 0 & 0 & 0 & 2d_3 \\ 0 & 0 & 2d_3 & 0 \end{bmatrix}, \tag{26}$$

when $d_1, d_2, d_3 > 0$ and $d_4 < 0$, and

$$\begin{bmatrix} 0 & 2d_1 & 0 & 0 \\ 2d_1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2d_3 \\ 0 & 0 & 2d_3 & 0 \end{bmatrix}, \tag{27}$$

when $d_1, d_3 > 0$ and $d_2, d_4 < 0$. Using the OCM for the $4 \times 4 \times 9$ array and taking advantage of the simple forms found for the $4 \times 4 \times 1$ orthogonal complement $\mathbf{D}$, (26) and (27), respectively, we have various simple forms for $\underline{\mathbf{X}}$. When the complement is $\mathbf{D}$, we have

$$\begin{aligned}&\left[\begin{array}{cccc|cccc|cccc|cccc|cccc|} 1&0&0&0&1&0&0&0&1&0&0&0&0&1&0&0&0&0&1&0 \\ 0&\alpha&0&0&0&0&0&0&0&0&0&0&1&0&0&0&0&0&0&0 \\ 0&0&0&0&0&0&\beta&0&0&0&0&0&0&0&0&0&1&0&0&0 \\ 0&0&0&0&0&0&0&0&0&0&0&\gamma&0&0&0&0&0&0&0&0 \end{array}\right. \\ &\quad\left.\begin{array}{cccc|cccc|cccc|cccc} 0&0&0&1&0&0&0&0&0&0&0&0&0&0&0&0 \\ 0&0&0&0&0&0&1&0&0&0&0&1&0&0&0&0 \\ 0&0&0&0&0&1&0&0&0&0&0&0&0&0&0&1 \\ 1&0&0&0&0&0&0&0&0&1&0&0&0&0&1&0 \end{array}\right]\end{aligned} \tag{28}$$

of weight 18. When the complement is (26), we have

$$\begin{aligned}&\left[\begin{array}{cccc|cccc|cccc|cccc|cccc|} 1&0&0&0&0&0&0&0&0&0&0&0&0&1&0&0&0&0&1&0 \\ 0&\alpha&0&0&0&0&0&0&0&0&0&0&1&0&0&0&0&0&0&0 \\ 0&0&0&0&0&0&1&0&0&0&0&0&0&0&0&0&1&0&0&0 \\ 0&0&0&0&0&0&0&0&0&0&0&1&0&0&0&0&0&0&0&0 \end{array}\right. \\ &\quad\left.\begin{array}{cccc|cccc|cccc|cccc} 0&0&0&1&0&0&0&0&0&0&0&0&\beta&0&0&0 \\ 0&0&0&0&0&0&1&0&0&0&0&1&0&0&0&0 \\ 0&0&0&0&0&1&0&0&0&0&0&0&0&0&0&1 \\ 1&0&0&0&0&0&0&0&0&1&0&0&0&0&1&0 \end{array}\right]\end{aligned} \tag{29}$$

of weight 17. When the complement is (27), we have

$$\begin{aligned}&\left[\begin{array}{cccc|cccc|cccc|cccc|cccc|} 1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&0 \\ 0&0&0&0&0&1&0&0&0&0&0&0&0&0&0&0&1&0&0&0 \\ 0&0&0&0&0&0&0&0&0&0&1&0&0&0&0&0&0&0&0&\alpha \\ 0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&0&\alpha&0 \end{array}\right. \\ &\quad\left.\begin{array}{cccc|cccc|cccc|cccc} 0&0&1&0&0&0&0&1&0&0&0&0&0&0&0&0 \\ 0&0&0&0&0&0&0&0&0&0&1&0&0&0&0&1 \\ 1&0&0&0&0&0&0&0&0&1&0&0&0&0&0&0 \\ 0&0&0&0&1&0&0&0&0&0&0&0&0&1&0&0 \end{array}\right]\end{aligned} \tag{30}$$

of weight 16. The conclusion is that, in general, a simplification of a $4 \times 4 \times 9$ symmetric slice array into a weight 18 simple array (28) is always possible. This result can be improved, when the signs of the eigenvalues of the orthogonal complement of $\underline{\mathbf{X}}$ permit, to a weight 17 or weight 16 array (29) or (30), respectively.

Next, we treat the $4 \times 4 \times 2$ case $\underline{\mathbf{X}} = [\mathbf{X}_1 | \mathbf{X}_2]$. Defining $\mathbf{M} = \mathbf{X}_1^{-1}\mathbf{X}_2$, three possibilities arise: either all eigenvalues of $\mathbf{M}$ are real, or $\mathbf{M}$ has one pair of complex eigenvalues, or $\mathbf{M}$ has two pairs of complex eigenvalues.

• **M has all eigenvalues real**

When all eigenvalues are real, $\underline{\mathbf{X}}$ has rank 4 [16]. As argued in the case of $3 \times 3 \times 2$ arrays when all eigenvalues are real, it is possible to perform a double diagonalization, followed by reducing the rank of each slice to be 3, so we can have the weight 6 array

$$\left[\begin{array}{cccc|cccc} 0 & 0 & 0 & 0 & \gamma & 0 & 0 & 0 \\ 0 & \alpha & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \beta & 0 & 0 & 0 & \delta & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 \end{array}\right]. \tag{31}$$

Another simple form that can be achieved using a procedure similar to the one that led to (20) is given by

$$\left[\begin{array}{cccc|cccc} \alpha & 0 & 0 & 0 & \gamma & 0 & 0 & 0 \\ 0 & \beta & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 \end{array}\right]. \tag{32}$$

Although (32) has weight 7, it will be useful in terms of the $4 \times 4 \times 8$ complement.

• **M has one pair of complex eigenvalues**

Let, in the eigenvalue decomposition $\mathbf{M} = \mathbf{KLK}^{-1}$, the real eigenvalues be $\mathbf{L}(1,1)$ and $\mathbf{L}(2,2)$. Consider matrix $\mathbf{S} = [\mathbf{k}_1 | \mathbf{k}_2 | \text{ real}(\mathbf{k}_3) | \text{imag}(\mathbf{k}_3)]$, where $\mathbf{k}_i$ is the ith column of $\mathbf{K}$. Then [18] we have

$$[\mathbf{S}'\mathbf{X}_1\mathbf{S} | \mathbf{S}'\mathbf{X}_2\mathbf{S}] = \left[\begin{array}{cccc|cccc} * & 0 & 0 & 0 & * & 0 & 0 & 0 \\ 0 & a & 0 & 0 & 0 & d & 0 & 0 \\ 0 & 0 & b & c & 0 & 0 & e & f \\ 0 & 0 & c & -b & 0 & 0 & f & -e \end{array}\right], \tag{33}$$

where $*$ denotes a nonzero entry. The pair of lower-right 3×3 submatrices have an already known form, see (21). Therefore, using here the same procedure used to simplify (21) applied to these blocks, we obtain a weight 7 symmetric simple form

$$\left[\begin{array}{cccc|cccc} \alpha & 0 & 0 & 0 & \gamma & 0 & 0 & 0 \\ 0 & \beta & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & -1 & 0 & 0 & 1 & 0 \end{array}\right], \tag{34}$$

similar to (32). In fact, both arrays lead to $4 \times 4 \times 8$ complements with the same pattern of (non)zeros.

• **M has two pairs of complex eigenvalues**

Rocci and Ten Berge [12] explain how to perform a slice mix of $\mathbf{X}_1$ and $\mathbf{X}_2$ such that for the new slices $\widetilde{\mathbf{X}}_1, \widetilde{\mathbf{X}}_2$ we have that $\widetilde{\mathbf{X}}_1^{-1}\widetilde{\mathbf{X}}_2$ has pure imaginary eigenvalues, so we will assume that $\underline{\mathbf{X}}$ is already in such form. Write the eigenvalue decomposition of $\mathbf{M} = \mathbf{KLK}^{-1}$ with $\mathbf{L}$ holding conjugate eigenvalues placed next to each other, and consider $\mathbf{S} = [\text{real}(\mathbf{k}_1) | \text{imag}(\mathbf{k}_1) | \text{real}(\mathbf{k}_3) | \text{imag}(\mathbf{k}_3)]$, where $\mathbf{k}_i$ is the ith column of $\mathbf{K}$. Then [18]

$$[\mathbf{S}'\mathbf{X}_1\mathbf{S} | \mathbf{S}'\mathbf{X}_2\mathbf{S}] = \left[\begin{array}{cccc|cccc} a & b & 0 & 0 & e & f & 0 & 0 \\ b & -a & 0 & 0 & f & -e & 0 & 0 \\ 0 & 0 & c & d & 0 & 0 & g & h \\ 0 & 0 & d & -c & 0 & 0 & h & -g \end{array}\right]. \tag{35}$$

Denote these slices by $\mathbf{Z}_1$ and $\mathbf{Z}_2$. It is clear that $\mathbf{Z}_1^{-1}\mathbf{Z}_2$ has the same eigenvalues as $\mathbf{M}$.

The next step consists of obtaining the eigenvalue decomposition $\mathbf{Z}_1 = \mathbf{K}_1\mathbf{L}_1\mathbf{K}_1'$. Notice that $\mathbf{Z}_1$ has two pairs of real eigenvalues differing only in signs. We shall prove next that $[\mathbf{K}_1'\mathbf{Z}_1\mathbf{K}_1|\mathbf{K}_1'\mathbf{Z}_2\mathbf{K}_1]$ has the symmetric form

$$\left[\begin{array}{cccc|cccc} * & 0 & 0 & 0 & 0 & * & 0 & 0 \\ 0 & * & 0 & 0 & * & 0 & 0 & 0 \\ 0 & 0 & * & 0 & 0 & 0 & 0 & * \\ 0 & 0 & 0 & * & 0 & 0 & * & 0 \end{array}\right] \tag{36}$$

if $\mathbf{L}_1$ holds the opposite eigenvalues placed next to each other, e.g., $\lambda_1, -\lambda_1, \lambda_2, -\lambda_2$. This form can be seen as related to (32) and (34), from the previous cases. We notice that the form of the first slice is obvious (it is $\mathbf{L}_1$), but the form of the second slice deserves further inspection.

We start by observing that the 2×2 diagonal blocks in $\mathbf{Z}_1$ and $\mathbf{Z}_2$ are proportional to orthonormal matrices. Therefore, we can write

$$\mathbf{Z}_1 = \begin{bmatrix} \gamma_1\mathbf{T}_1 & \mathbf{0} \\ \mathbf{0} & \gamma_2\mathbf{T}_2 \end{bmatrix}, \quad \mathbf{Z}_2 = \begin{bmatrix} \gamma_3\mathbf{T}_3 & \mathbf{0} \\ \mathbf{0} & \gamma_4\mathbf{T}_4 \end{bmatrix} \tag{37}$$

with $\mathbf{T}_1, \ldots, \mathbf{T}_4$ symmetric and orthonormal, with eigenvalues 1 and -1. Then

$$\mathbf{Z}_1^{-1}\mathbf{Z}_2 = \begin{bmatrix} \gamma_1^{-1}\gamma_3\mathbf{T}_1\mathbf{T}_3 & \mathbf{0} \\ \mathbf{0} & \gamma_2^{-1}\gamma_4\mathbf{T}_2\mathbf{T}_4 \end{bmatrix}. \tag{38}$$

First, consider the upper-left 2×2 block. Define $\mathbf{G} = \mathbf{T}_1\mathbf{T}_3$ (so $\mathbf{T}_3 = \mathbf{T}_1\mathbf{G}$); $\mathbf{G}$ is orthonormal with pure imaginary eigenvalues. Consider its eigenvalue decomposition $\mathbf{G} = \mathbf{K}_G\mathbf{L}_G\mathbf{K}_G^{-1}$ with $\mathbf{L}_G = \mathrm{diag}(-iu, iu)$, then $\mathbf{G}^2 = -u^2\mathbf{I}_2$. This implies that $\det(\mathbf{G}^2) = u^4$, but we also have that $\det(\mathbf{G}^2) = \det(\mathbf{G}'\mathbf{G}) = \det(\mathbf{I}_2) = 1$, and so $u = \pm 1$. Hence $\mathbf{G}^2 = -\mathbf{I}_2$. From this equality and the orthonormality of $\mathbf{G}$ we get that $\mathbf{G} = -\mathbf{G}'$, so $\mathbf{G}$ is a skew matrix. Combining this fact with the orthonormality of $\mathbf{G}$ allows to conclude that $\mathbf{G} = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}$, up to sign. Next, since $\mathbf{T}_1$ has eigenvalues 1 and -1, we can write the eigenvalue decomposition $\mathbf{T}_1 = \mathbf{K}_{\mathbf{T}_1}\mathbf{L}_{\mathbf{T}_1}\mathbf{K}'_{\mathbf{T}_1}$ with $\mathbf{L}_{\mathbf{T}_1} = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$ and $\mathbf{K}_{\mathbf{T}_1}$ orthonormal. From this we have $\mathbf{K}'_{\mathbf{T}_1}\mathbf{T}_1\mathbf{K}_{\mathbf{T}_1} = \mathbf{L}_{\mathbf{T}_1}$ (diagonal) and

$$\begin{aligned} \mathbf{K}'_{\mathbf{T}_1}\mathbf{T}_3\mathbf{K}_{\mathbf{T}_1} &= \mathbf{K}'_{\mathbf{T}_1}\mathbf{T}_1\mathbf{G}\mathbf{K}_{\mathbf{T}_1} = \mathbf{K}'_{\mathbf{T}_1}\mathbf{K}_{\mathbf{T}_1}\mathbf{L}_{\mathbf{T}_1}\mathbf{K}'_{\mathbf{T}_1}\mathbf{G}\mathbf{K}_{\mathbf{T}_1} \\ &= \mathbf{L}_{\mathbf{T}_1}\mathbf{K}'_{\mathbf{T}_1}\mathbf{G}\mathbf{K}_{\mathbf{T}_1} = \pm\mathbf{L}_{\mathbf{T}_1}\mathbf{G} = \pm\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \end{aligned}$$

(the second last equality is because $\mathbf{K}'_{\mathbf{T}_1}\mathbf{G}\mathbf{K}_{\mathbf{T}_1}$ is orthonormal and skew, and therefore it equals $\mathbf{G}$ up to sign). The same process can be applied to the lower-right 2×2 blocks of $\mathbf{Z}_1$ and $\mathbf{Z}_2$. We can conclude that if we pre and postmultiply the slices of the array $[\mathbf{Z}_1|\mathbf{Z}_2]$ by $\mathbf{K}_1'$ and $\mathbf{K}_1$, respectively, where $\mathbf{K}_1 = \begin{bmatrix} \mathbf{K}_{\mathbf{T}_1} & \mathbf{0} \\ \mathbf{0} & \mathbf{K}_{\mathbf{T}_2} \end{bmatrix}$ is the matrix of eigenvectors of $\mathbf{Z}_1$, then

$$[\mathbf{K}_1'\mathbf{Z}_1\mathbf{K}_1|\mathbf{K}_1'\mathbf{Z}_2\mathbf{K}_1] = \left[\begin{array}{cccc|cccc} \gamma_1 & 0 & 0 & 0 & 0 & \delta_1\gamma_3 & 0 & 0 \\ 0 & -\gamma_1 & 0 & 0 & \delta_1\gamma_3 & 0 & 0 & 0 \\ 0 & 0 & \gamma_2 & 0 & 0 & 0 & 0 & \delta_2\gamma_4 \\ 0 & 0 & 0 & -\gamma_2 & 0 & 0 & \delta_2\gamma_4 & 0 \end{array}\right] \tag{39}$$

with $\delta_1 = \pm 1, \delta_2 = \pm 1$.

We can use the simple forms that were deduced for symmetric $4 \times 4 \times 2$ arrays to compute simple forms for the $4 \times 4 \times 8$ case using the OCM. So, depending on which situation we have for $\underline{\mathbf{X}}^c$, we may have $\underline{\mathbf{H}}^c$ as in (32), (34) or (39). The first two cases lead to a complement of weight 18 with the following slices:

$$\left[\begin{array}{cccc|cccc|cccc|cccc|} -2\beta & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 2\alpha & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & \beta\gamma & 0 & 0 & -\beta & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \beta\gamma & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\beta\delta & 0 & 0 & 0 & 0 \end{array}\right.$$

$$\left.\begin{array}{cccc|cccc|cccc|cccc}
0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0
\end{array}\right], \tag{40}$$

where α, β, and γ have the same meaning as in (32) and (34), and $\delta = 1$ in the first case and -1 in the second case. The third case leads to a complement of the form

$$\left[\begin{array}{cccc|cccc|cccc|cccc}
1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & -\gamma_1\gamma_2^{-1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \alpha \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \gamma_1\gamma_2^{-1} & 0 & 0 & \alpha & 0
\end{array}\right|$$
$$\left.\begin{array}{cccc|cccc|cccc|cccc}
0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0
\end{array}\right], \tag{41}$$

with $\alpha = -\delta_1\delta_2^{-1}\gamma_3\gamma_4^{-1}$, again of weight 18. The overall conclusion is that a symmetric $4 \times 4 \times 8$ array can almost surely be simplified into one out of two weight 18 arrays.

8. Applications to typical rank

Results concerning typical rank for several symmetric slice arrays are presented in Ten Berge et al. [16]. Using the simplicity results presented above, we can now further clarify some of the results deduced in [16]. We shall do this by revisiting the typical rank issue (over the field of real numbers) for $3 \times 3 \times 4$ and the $3 \times 3 \times 5$ array formats, when slices are symmetric.

• **Symmetric slice** $3 \times 3 \times 4$ **arrays**

We proved that a possible simple form for $3 \times 3 \times 4$ symmetric slice arrays that works almost always is given by (25). Ten Berge et al. [16] have proven that $3 \times 3 \times 4$ symmetric slice arrays have typical rank $\{4, 5\}$. The proof consists of constructing a rank four solution for a randomly sampled symmetric slice array, and determining under which conditions we need a rank five solution. Here we shall do the same, this time using (25). Our purpose is to put in evidence how helpful simple forms can be to study the rank of an array.

We start by unfolding the array and vectorizing its frontal slices, so we get $\mathbf{X}_{\mathrm{Vec}} = [\mathrm{Vec}(\mathbf{X}_1)|\cdots|\mathrm{Vec}(\mathbf{X}_4)]$. Noting that a CP decomposition can be written in the form $\mathbf{X}_{\mathrm{Vec}} = (\mathbf{A} \bullet \mathbf{B})\mathbf{C}'$, where $\bullet$ stands for the Khatri-Rao product, it can be concluded that a rank 4 solution exists if and only if there exists a Khatri–Rao basis $\mathbf{A} \bullet \mathbf{B}$ which generates $\mathbf{X}_{\mathrm{Vec}}$. Equivalently, we may solve $\mathbf{X}_{\mathrm{Vec}}\mathbf{W} = \mathbf{A} \bullet \mathbf{B}$, with $\mathbf{W} = (\mathbf{C}')^{-1}$. The problem sums up to finding four linearly independent vectors $\mathbf{w}$ (columns of $\mathbf{W}$) such that $\mathbf{X}_{\mathrm{Vec}}\mathbf{w}$ is the Kronecker product of two vectors (columns of $\mathbf{A}$ and $\mathbf{B}$), which may be rescaled to be $\mathbf{a} = [1\ a_1\ a_2]'$ and $\mathbf{b} = [1\ b_1\ b_2]'$, respectively, for scalars a_1, a_2, b_1 and b_2. We have

$$\mathbf{X}_{\mathrm{Vec}} = \begin{bmatrix} 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ \alpha & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & \delta\alpha & 0 & 0 \end{bmatrix} \quad \textit{and} \quad \mathbf{a} \otimes \mathbf{b} = \begin{bmatrix} 1 \\ b_1 \\ b_2 \\ a_1 \\ a_1 b_1 \\ a_1 b_2 \\ a_2 \\ a_2 b_1 \\ a_2 b_2 \end{bmatrix}. \tag{42}$$

Solving $\mathbf{X}_{\mathrm{Vec}}\mathbf{w} = \mathbf{a} \otimes \mathbf{b}$ for $\mathbf{w}$ yields $\mathbf{a} = \mathbf{b}$ and $\mathbf{w} = [\alpha^{-1}\ b_1^2\ \delta\alpha^{-1}\ b_2^2\ b_1\ b_2]'$. There are two equations left, $b_1 b_2 = 0$ and $b_1^2 + \delta b_2^2 = \alpha$. The last two equations have four solutions if and only if $\delta = 1$ and α is positive, being the solutions $b_1 = 0, b_2 = \pm\sqrt{\alpha}$ and $b_1 = \pm\sqrt{\alpha}, b_2 = 0$. With this we already have

$$\mathbf{A} = \mathbf{B} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 0 & 0 & \sqrt{\alpha} & -\sqrt{\alpha} \\ \sqrt{\alpha} & -\sqrt{\alpha} & 0 & 0 \end{bmatrix}. \tag{43}$$

We find $\mathbf{C}$ as $\mathbf{C} = (\mathbf{W}^{-1})'$, which is given by

$$\mathbf{C} = \begin{bmatrix} 0 & 0 & 0.5 & 0.5 \\ 0.5 & 0.5 & 0 & 0 \\ 0 & 0 & 0.5\sqrt{\alpha^{-1}} & -0.5\sqrt{\alpha^{-1}} \\ 0.5\sqrt{\alpha^{-1}} & -0.5\sqrt{\alpha^{-1}} & 0 & 0 \end{bmatrix}. \tag{44}$$

We conclude that, when $\delta = 1$ and $\alpha > 0$, a unique rank four decomposition of $\underline{\mathbf{X}}$ is given by $\mathbf{X}_k = \mathbf{A}\mathbf{C}_k\mathbf{A}'$, $k = 1, \ldots, 4$, with $\mathbf{A}$ and $\mathbf{C}$ given by (43) and (44).

When $\delta = -1$ or $\alpha < 0$, the rank of $\underline{\mathbf{X}}$ is larger than 4. A rank 5 solution can be constructed as follows. Consider array $\underline{\mathbf{X}}$ temporarily augmented with a fifth slice $\mathbf{X}_5 = \mathrm{diag}(-\delta\alpha^2, \delta\alpha, \alpha)$, and define $\mathbf{X}_{\mathrm{aug}} = [\mathrm{Vec}(\mathbf{X}_1)|\ldots|\,\mathrm{Vec}(\mathbf{X}_5)]$. Proceeding as before, it is possible to find $\mathbf{A}(3 \times 5)$ and $\mathbf{C}_{\mathrm{aug}}(5 \times 5)$ such that $\mathbf{X}_{\mathrm{aug}} = (\mathbf{A}\bullet\mathbf{A})\mathbf{C}'_{\mathrm{aug}}$. We find $\mathbf{C}$ by eliminating the fifth row of $\mathbf{C}_{\mathrm{aug}}$. There are many solutions possible. If we settle for

$$\mathbf{A} = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ 0 & 0 & 1 & -1 & 0 \\ 1 & -1 & 0 & 0 & 0 \end{bmatrix}, \tag{45}$$

then $\mathbf{C}$ will be

$$\mathbf{C} = \begin{bmatrix} 0 & 0 & 0.5\alpha & 0.5\alpha & 1-\alpha \\ 0.5\delta\alpha & 0.5\delta\alpha & 0 & 0 & 1-\delta\alpha \\ 0 & 0 & 0.5 & -0.5 & 0 \\ 0.5 & -0.5 & 0 & 0 & 0 \end{bmatrix}. \tag{46}$$

This is a closed form solution for $3 \times 3 \times 4$ symmetric slice arrays of rank 5.

The derivation above, based on the simplicity pattern (25), has enabled us to greatly simplify the rank analysis of $3 \times 3 \times 4$ symmetric slice arrays, compared to [16]. All it takes to determine the rank of such an array is seeing whether or not α and δ of (25) are positive or not. This is easier than evaluating the roots of a certain fourth degree polynomial to see if they are real and distinct, [16]. In fact, that fourth degree polynomial has now been reduced to $(\lambda^2 - \alpha)(\lambda^2 - \delta\alpha)$. In addition, finding a rank 5 solution when a rank four solution fails is now also trivially easy, as is clear from (45) and (46).

• **Symmetric slice $3 \times 3 \times 5$ arrays**

In [16] it is proven that $3 \times 3 \times 5$ symmetric slice arrays have typical rank {5,6}. We proved that a possible simple form is given by (14). We can proceed as done before for the $3 \times 3 \times 4$ situation. Construct $\mathbf{X}_{\mathrm{Vec}} = [\mathrm{Vec}(\mathbf{X}_1)|\cdots|\mathrm{Vec}(\mathbf{X}_5)]$. For a rank 5 solution to exist we need to find a Khatri–Rao basis which generates $\mathbf{X}_{\mathrm{Vec}} = (\mathbf{A} \bullet \mathbf{B})\mathbf{C}'$. This is the same as solving $\mathbf{X}_{\mathrm{Vec}}\mathbf{W} = \mathbf{A} \bullet \mathbf{B}$, with $\mathbf{W} = (\mathbf{C}')^{-1}$. Denoting rescaled columns of $\mathbf{A}$ and $\mathbf{B}$ by $\mathbf{a} = [1\ a_1\ a_2]'$ and $\mathbf{b} = [1\ b_1\ b_2]'$ respectively, for scalars a_1, a_2, b_1 and b_2, we get

$$\mathbf{X}_{\mathrm{Vec}} = \begin{bmatrix} 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ \alpha & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & \beta & 0 & 0 & 0 \end{bmatrix} \quad \text{and} \quad \mathbf{a} \otimes \mathbf{b} = \begin{bmatrix} 1 \\ b_1 \\ b_2 \\ a_1 \\ a_1 b_1 \\ a_1 b_2 \\ a_2 \\ a_2 b_1 \\ a_2 b_2 \end{bmatrix}. \tag{47}$$

Solving $\mathbf{X}_{\mathrm{Vec}}\mathbf{w} = \mathbf{a} \otimes \mathbf{b}$ for $\mathbf{w}$ implies that $\mathbf{a} = \mathbf{b}$ and $\mathbf{w} = [\alpha^{-1}b_1^2\ \beta^{-1}b_2^2\ b_1\ b_2\ b_1b_2]'$. There is one condition that remains to be solved, which is equation $\alpha^{-1}b_1^2 + \beta^{-1}b_2^2 = 1$. This equation implies that there is a solution (and therefore a rank 5 decomposition) if and only if $\alpha > 0$ and/or $\beta > 0$. When the latter condition is satisfied, we can deduce closed form solutions. There is an infinite number of solutions, of which the ones presented next are only a possibility:

- if $\alpha > 0$ and $\beta > 0$:

$$\mathbf{A} = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ 0 & 0 & \sqrt{\alpha} & -\sqrt{\alpha} & 0.5\sqrt{\alpha} \\ \sqrt{\beta} & -\sqrt{\beta} & 0 & 0 & \sqrt{0.75\beta} \end{bmatrix}, \tag{48}$$

$$\mathbf{C} = \begin{bmatrix} 0 & 0 & 0.5 & 0.5 & 0 \\ 0.5 & 0.5 & 0 & 0 & 0 \\ 0 & 0 & 0.5\sqrt{\alpha^{-1}} & -0.5\sqrt{\alpha^{-1}} & 0 \\ 0.5\sqrt{\beta^{-1}} & -0.5\sqrt{\beta^{-1}} & 0 & 0 & 0 \\ -2(\sqrt{0.75}+0.75)k & 2(\sqrt{0.75}-0.75)k & -1.5k & 0.5k & 4k \end{bmatrix}, \tag{49}$$

with $k = \sqrt{3^{-1}\alpha^{-1}\beta^{-1}}$.

- if $\alpha > 0$ and $\beta < 0$:

$$\mathbf{A} = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ \sqrt{\alpha} & -\sqrt{\alpha} & \sqrt{2\alpha} & \sqrt{2\alpha} & -\sqrt{2\alpha} \\ 0 & 0 & \sqrt{-\beta} & -\sqrt{-\beta} & \sqrt{-\beta} \end{bmatrix} \tag{50}$$

and

$$\mathbf{C} = \begin{bmatrix} 0.5 & 0.5 & 0 & 0 & 0 \\ 1+\sqrt{0.5} & 1-\sqrt{0.5} & -0.5 & -0.5 & 0 \\ 0.5\sqrt{\alpha^{-1}} & -0.5\sqrt{\alpha^{-1}} & 0 & 0 & 0 \\ \sqrt{-0.5\beta^{-1}} & -\sqrt{-0.5\beta^{-1}} & 0 & -0.5\sqrt{-\beta^{-1}} & 0.5\sqrt{-\beta^{-1}} \\ -0.5\sqrt{-\alpha^{-1}\beta^{-1}} & 0.5\sqrt{-\alpha^{-1}\beta^{-1}} & 0.5\sqrt{-0.5\alpha^{-1}\beta^{-1}} & 0 & -0.5\sqrt{-0.5\alpha^{-1}\beta^{-1}} \end{bmatrix}.$$

When the rank is 6, that is, when $\alpha < 0$ and $\beta < 0$, a simple decomposition based on [11] is the following:

$$\mathbf{A} = \begin{bmatrix} 1 & 0 & 0 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 1 & 1 & 0 \end{bmatrix}, \mathbf{C} = \begin{bmatrix} 1 & \alpha & 0 & 0 & 0 & 0 \\ 1 & 0 & \beta & 0 & 0 & 0 \\ -1 & -1 & 0 & 0 & 0 & 1 \\ -1 & 0 & -1 & 0 & 1 & 0 \\ 0 & -1 & -1 & 1 & 0 & 0 \end{bmatrix}. \tag{51}$$

9. Maximal simplicity

We have presented simple forms for some symmetric slice arrays. A natural question that arises concerns the optimality of the simple targets, described in terms of minimal weight. That is, have the simple forms we presented the maximal simplicity possible?

For some cases it is possible to prove at once that the simple forms presented have minimal weight. For instance, the weight 9 form (8) for the $3 \times 3 \times 6$ symmetric slice array has maximal simplicity. In fact, if a simple form $\underline{\mathbf{H}}$ with weight less than 9 were possible, then it would have at least four slices of weight 1. The symmetry of these four slices implies that the weights must be placed in the diagonal of each slice, which leads to the conclusion that $\underline{\mathbf{H}}$ has linearly dependent slices. So weight 9 is associated to the maximal simplicity possible for $3 \times 3 \times 6$ symmetric slice arrays with linearly independent slices, or more generally, weight I^2 is the optimal weight for $I \times I \times K_{\max}$ symmetric slice arrays with linearly independent slices.

The weight of an array is an upper bound to the rank of an array. Usually this bound is larger than the rank, but in cases of low order it might give some insight regarding maximal simplicity. For example, it was shown that the $2 \times 2 \times 2$ symmetric slice array $\underline{\mathbf{X}}$ can be transformed into the simple form with weight 4 given by (11), and when $\alpha < 0$ the weight 2 simple target given by (12) is also possible. It is well known that $\underline{\mathbf{X}}$ has rank 2 when $\alpha < 0$ and rank 3 when $\alpha > 0$. This immediately implies that (12) has maximal simplicity when $\alpha < 0$, since in this situation the weight equals the rank. On the other hand, it is easy to show that there is no slice mix of (11) with rank 1 when $\alpha > 0$, which implies that no Tucker transformations applied to (11) can lead to slices of rank 1. This means that weight 4 is the minimal possible in this case.

The OCM can also be used in this context. Consider, for instance, the $3 \times 3 \times 5$ symmetric slice array. We showed that a randomly generated array of this order can always be simplified into a weight 10 simple array (14), and in some situations a weight 9 array is also possible, see (15). The question to answer at the moment is: is it possible to have a simpler (smaller weight) target? Assuming that it is possible, we shall consider all simpler targets available. Noting that weight 6 or less would imply linearly dependent slices, we are left with the following two types of arrays (without loss of generality):

$$\underline{\mathbf{H}}_1 = \left[\begin{array}{ccc|ccc|ccc|ccc|ccc} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 \end{array}\right] \tag{52}$$

and

$$\underline{\mathbf{H}}_2 = \left[\begin{array}{ccc|ccc|ccc|ccc|ccc} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \end{array}\right]. \tag{53}$$

Arrays (52) and (53) admit the following orthogonal complements, respectively,

$$\underline{\mathbf{H}}_1^{\mathbf{c}} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad \underline{\mathbf{H}}_2^{\mathbf{c}} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}. \tag{54}$$

When an orthogonal complement set contains a single symmetric matrix that is rescaled to unit sums of squares, and rescaled to have a certain nonzero element positive (viz. the element (1,1) in $\underline{\mathbf{H}}_1^{\mathbf{c}}$, and the element (2,3) in $\sqrt{.5}\underline{\mathbf{H}}_2^{\mathbf{c}}$), that complement matrix depends continuously on the given array. Moreover, the determinant of a square matrix of order n is a real valued analytic function. Since the determinant of orthogonal complement matrices of $3 \times 3 \times 5$ symmetric slice arrays is not identically zero, we can conclude that such matrices have determinant nonzero almost surely [2]. This implies that both complements in (54) arise with probability zero, and so the simple forms (52) and (53) may be discarded. It can be concluded that $3 \times 3 \times 5$ arrays admit simple forms with weight less than 9 with probability zero.

It was proved in this paper that for $3 \times 3 \times 2$ symmetric slice arrays $\underline{\mathbf{X}} = [\mathbf{X}_1|\mathbf{X}_2]$ a weight 5 simple form is always possible (arrays (20) or (24)), and in some situations weight 4 is possible (array (16)). A simple form with weight 3 is not possible, because it can be seen that no slice mix from (20) or (24) will ever lead to a rank 1 matrix. Therefore, the maximal simplicity for $3 \times 3 \times 2$ symmetric slice arrays is weight 4. Furthermore, when $\mathbf{X}_1^{-1}\mathbf{X}_2$ has complex eigenvalues it is not possible to improve the weight 5 simple form (24), since it can be seen that any weight 4 symmetric slice array has real generalized eigenvalues.

Finally, consider the $3 \times 3 \times 4$ symmetric slice arrays. We were able to simplify these arrays into (25), which has weight 8. For this result to have maximal simplicity, we need to ensure that weight 7 or less can not occur with positive probability. It can be seen that any simple form of weight 6 or less with at least three slices of rank 1 has a $3 \times 3 \times 2$ orthogonal complement spanned by two slices that do not admit a linear combination of rank 3, which is an event of probability 0. Also, simple forms with weight 6 and only two rank 1 slices happen with probability zero, since their orthogonal complement spaces are spanned by pairs of slices with joint weight 3. So we need to only focus on weight 7 targets. There are two possible types of targets:

- We can have exactly two slices of rank 1, such as in array $\underline{\mathbf{H}}_1$:

$$\underline{\mathbf{H}}_1 = \left[\begin{array}{ccc|ccc|ccc|ccc} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \alpha & 1 & 0 & 0 \end{array}\right]. \tag{55}$$

There are 18 different possibilities in total, but the reasoning to be presented to only this example applies to all. Notice that $\underline{\mathbf{H}}_1$ is impossible almost surely, because its orthogonal complement $\underline{\mathbf{H}}_1^{\mathbf{c}}$,

$$\underline{\mathbf{H}}_1^{\mathbf{c}} = \left[\begin{array}{ccc|ccc} 0 & 0 & 0 & 0 & -\alpha & 0 \\ 0 & 0 & 1 & -\alpha & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 2 \end{array}\right] \tag{56}$$

is a $3 \times 3 \times 2$ symmetric slice array such that any slice mix will lead to three repeated real generalized eigenvalues, an event of probability zero. In some of the cases the orthogonal complement cannot even lead to full rank matrices by linear combination of the slices, which is also an event of probability zero.
- We can have exactly one slice of rank 1. One possibility, given by

$$\underline{\mathbf{H}}_2 = \left[\begin{array}{ccc|ccc|ccc|ccc} 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 \end{array}\right] \tag{57}$$

can be ruled out since its complement $\underline{\mathbf{H}}_2^{\mathbf{c}}$,

$$\underline{\mathbf{H}}_2^{\mathbf{c}} = \left[\begin{array}{ccc|ccc} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{array}\right] \tag{58}$$

is a $3 \times 3 \times 2$ symmetric slice array with only weight 2. There are nine possibilities left. Six of them, such as $\underline{\mathbf{H}}_3$,

$$\underline{\mathbf{H}}_3 = \left[\begin{array}{ccc|ccc|ccc|ccc} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 \\ 0 & a & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \end{array}\right] \tag{59}$$

lead to an orthogonal complement such that any slice mix with at least one invertible slice will lead to a pair of repeated real generalized eigenvalues, which is an event of probability zero. The remaining three possibilities have orthogonal complements that again do not admit full rank matrices as linear combinations of their slices, which is an event of probability zero.

The conclusion is that weight 8 is indeed the maximal simplicity almost surely for $3 \times 3 \times 4$ symmetric slice arrays.

10. Results from simulations: the SIMPLIMAX procedure

For many situations it is not easy to find simple forms, or assess maximal simplicity. When formal proofs might be difficult, one can still use simulation as an informal way of making, reinforcing or refuting one's hypotheses. Kiers [6] has developed a procedure called SIMPLIMAX, which finds oblique rotations that give the minimum sum of squares for a previously specified number m of entries for the rotated array. It is not known *a priori* which entries will be the smallest ones, so the algorithm will internally solve this issue. This has the side effect of SIMPLIMAX finding locally optimal solutions. This problem can be circumvented by using a large number of randomly started runs of the algorithm. An adapted version of SIMPLIMAX allows to fix, in advance, the position of the m entries whose sum of squares we intend to minimize. We shall refer to this as the fixed version of SIMPLIMAX, in contrast with the not fixed version of the algorithm.

SIMPLIMAX had a crucial role in the research that led to the present paper. The *modus operandi* was usually the following: for an array order for which we were interested in finding simple forms, we randomly generated a family of 30 such arrays, fixed some values for m, and ran the not fixed algorithm using MATLAB. A rotation was considered "successful" when the sum of squares of the m smallest elements was below a fixed threshold (we settled for 10^{-15}). For each array, we repeated the algorithm with a random different starting configuration (to avoid locally optimal solutions) to a maximum of 150 tries, unless a successful solution was found meanwhile. When we had found an interesting simple form to look at, we used fixed SIMPLIMAX to test it directly (again 30 randomly sampled arrays, 150 tries for each array). This gave us empirical probabilities of success for the targets at hand. This could be done for several targets with equal weight, as a way of comparing performances.

Most of the rotations to simplicity that we proved in this paper for arrays with 3×3 or 4×4 symmetric slices were first suggested to us by SIMPLIMAX. Moreover, maximal simplicity was also inspected. For each array order we examined, we ran not fixed SIMPLIMAX for 100 randomly generated arrays, aiming for targets with smaller weight than the simple forms we present. The results concerning orders $3 \times 3 \times K$ for $K = 2, 4, 5$ were consistent with the maximal simplicity we proved in this paper. For the arrays with 4×4 symmetric slices we considered, simulations indicate that weight 18 seems to be the maximal simplicity to expect for $K = 8$ slices. As for $4 \times 4 \times 9$ symmetric slice arrays, simulations seem to indicate that weight less than 16 does not happen. Moreover, the situations for which weight 18 and 17 simple forms (28) and (29) were developed do not seem to admit simpler forms.

11. Discussion

We have worked under the assumption that the arrays are randomly sampled from a continuous distribution, with the constraint of symmetry in the frontal slices. This means that we have ignored cases that arise with probability zero. However, one may question the "random" nature of a core array arising from a 3PCA procedure, as it is a product of an iterative algorithm. As Rocci and Ten Berge [12, p. 362] argue, "…we cannot infer that simplicity transformations which work almost surely for random arrays will also work for Tucker-3 core arrays. Fortunately, all Tucker-3 core arrays encountered so far do seem to behave as if randomly sampled from a continuous distribution, and do allow transformations to simplicity …". Still, a formal proof for this is lacking.

The results of this paper have direct implications for the possibility of simplifying core arrays in Tucker 3-way PCA. However, the realm of possible applications is more general. Matrix theory on the simultaneous reduction of pairs of matrices to sparse forms is abundant, but results for more than two matrices seem absent. The present paper explores the possibilities of filling this gap. For instance, it has been shown that $3 \times 3 \times 4$ arrays of symmetric slices can almost surely be reduced to a form where each of the four slices has weight 2. This is an extension of matrix theory that will be of interest beyond the realm of Tucker-3 PCA.

References

[1] J.D. Carroll, J.J. Chang, Analysis of individual differences in multidimensional scaling via an n-way generalization of Eckart–Young decomposition, Psychometrika 35 (1970) 283–319.
[2] F.M. Fisher, The Identification problem in Econometrics, McGraw-Hill, New York, 1966.
[3] R.A. Harshman, Foundations of the PARAFAC procedure: models and conditions for an "explanatory" multi-model factor analysis, University of California at Los Angeles. UCLA Working Papers in Phonetics, vol. 16, 1970, pp. 1–84.
[4] R.A. Harshman, Determination and proof of minimum uniqueness conditions for PARAFAC1, University of California at Los Angeles. UCLA Working Papers in Phonetics, vol. 22, 1972, pp. 111–117.
[5] H.A.L. Kiers, TUCKALS core rotations and constrained TUCKALS modeling, Stat. Appl. 4 (1992) 659–667.
[6] H.A.L. Kiers, Three-way SIMPLIMAX for oblique rotation of the three-mode factor analysis core to simple structure, Comput. Stat. Data Anal. 28 (1998) 307–324.
[7] P.M. Kroonenberg, J. de Leeuw, Principal component analysis of three-mode data by means of alternating least squares, Psychometrika 45 (1980) 69–97.
[8] J.B. Kruskal, Three-way arrays: Rank and uniqueness of trilinear decompositions, with applications to arithmetic complexity and statistics, Linear Algebra Appl. 18 (1977) 95–138.

[9] J.B. Kruskal, Rank, decomposition, and uniqueness for 3-way and *N*-way arrays, in: R. Coppi, S. Bolasco (Eds.), Multiway Data Analysis, North-Holland, Amsterdam, 1989, pp. 7–18.
[10] T. Murakami, J.M.F. Ten Berge, H.A.L. Kiers, A case of extreme simplicity of the core matrix in three-mode principal components analysis, Psychometrika 63 (1998) 255–261.
[11] R. Rocci, J.M.F. Ten Berge, A simplification of a result by Zellini on the maximal rank of symmetric three-way arrays, Psychometrika 59 (1994) 377–380.
[12] R. Rocci, J.M.F. Ten Berge, Transforming three-way arrays to maximal simplicity, Psychometrika 67 (2002) 351–365.
[13] J.M.F. Ten Berge, H.A.L. Kiers, Simplicity of core arrays in three-way principal component analysis and the typical rank of $p \times q \times 2$ arrays, Linear Algebra Appl. 294 (1999) 169–179.
[14] J.M.F. Ten Berge, The typical rank of tall three-way arrays, Psychometrika 65 (2000) 525–532.
[15] J.M.F. Ten Berge, H.A.L. Kiers, T. Murakami, R. van der Heijden, Transforming three-way arrays to multiple orthonormality, J. Chem. 14 (2000) 275–284.
[16] J.M.F. Ten Berge, N.D. Sidiropoulos, R. Rocci, Typical rank and Indscal dimensionality for symmetric three-way arrays of order $I \times 2 \times 2$ or $I \times 3 \times 3$, Linear Algebra Appl. 388 (2004) 363–377.
[17] L.R. Tucker, Some mathematical notes on three-mode factor analysis, Psychometrika 31 (1966) 279–311.
[18] F. Uhlig, A canonical form for a pair of real symmetric matrices that generate a nonsingular pencil, Linear Algebra Appl. 14 (1976) 189–209.